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N-P pairing in nuclei

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Abstract

Variational wavefunctions for treating N-P pairing in the $T = 1$ and $T = 0$ channels are presented. Alpha-like correlations are explicitly included in the wavefunctions and arbitrary single-particle energy level spacings are allowed. A triple projection before variation procedure is used to obtain these wavefunctions. Taking a model system with equally spaced single-particle levels, several features of nuclei near the $N = Z$ line are calculated. A new type of multiple degeneracy is found in nuclei near the $N = Z$ line.

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In a typical heavy nucleus, because of the substantial neutron excess, neutrons occupy single particle orbitals in a shell with a principal quantum number one larger than that of the protons. This difference in Fermi levels suppresses the correlations in low-lying states arising from N-P pairing. For nuclides near the $N = Z$ line, however, N-P pairing effects are important and an interesting pattern of correlations develops. Such correlations have been studied in the framework of extended quasi-particle approximations [1–5]. See Ref. [4] for an excellent guide to the to the early work. A second approach based on exact solutions of the degenerate model has also played an important role in understanding N-P pairing [6–10]. With the possibility of constructing a Rare Isotope Accelerator on the horizon, there is a renewed interest in this problem. A RIA facility would make spectroscopic studies near the $N = Z$ line feasible for heavier nuclides. In heavier nuclei, single particle level densities will be greater and pairing effects might be more apparent. There is a substantial amount

of ongoing work in both the extended quasi-particle approach [11–13] and in the degenerate model approach [14,15].

In this Letter, we take a different approach to N-P pairing. We construct wavefunctions that take the two neutron-two proton ‘alpha particle’ correlations explicitly into account. A need to find an effective way to take this correlation into account has been emphasized [15] in degenerate model studies. A second feature of our approach is triple projection before variation. In addition to the exact projection of both proton and neutron particle numbers, we project exactly the number parity of the $T = 0$ and $T = 1$ N-P pairs. Number parity projection is a first step to full isospin projection. We develop a treatment of excited states using amplitude interchanges combined with configuration interaction calculations.

The pairing force, considered here, includes N-N, P-P and N-P pairing, with both $T = 0$ and $T = 1$ components. Each of the Nilsson levels accommodates two protons and two neutrons. The Hamiltonian is

$$H = \sum_{k>0} \varepsilon_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k} + b_k^\dagger b_k + b_{-k}^\dagger b_{-k})$$

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$$\begin{aligned}
& - \sum_{i,j} G_{i,j}^{T=1} [A_i^\dagger A_j + B_i^\dagger B_j + C_i^\dagger C_j] \\
& - \sum_{i,j} G_{i,j}^{T=0} D_i^\dagger D_j,
\end{aligned} \quad (1)$$

where $a_k^\dagger (b_k^\dagger)$ denotes a neutron (proton) creation operator; $A_i^\dagger = (a_i^\dagger a_{-i}^\dagger)$ and $B_i^\dagger = (b_i^\dagger b_{-i}^\dagger)$. The $T = 1$ N-P pair creation operator is

$$C_i^\dagger = \frac{1}{\sqrt{2}} [a_i^\dagger b_{-i}^\dagger + a_{-i}^\dagger b_i^\dagger]$$

and the $T = 0$ N-P pair creation operator is

$$D_i^\dagger = \frac{i}{\sqrt{2}} [a_i^\dagger b_{-i}^\dagger - a_{-i}^\dagger b_i^\dagger].$$

Our ordering convention is to put neutron creation operators before proton creation operators in the C^\dagger and D^\dagger operators that appear in the Hamiltonian and in the wavefunctions. Therefore, we define the proton wavefunction with positive j_z as the negative of the equivalent neutron wavefunction to retain the usual plus sign in C^\dagger . D^\dagger is purely imaginary.

Our variational wavefunction is a product form

$$\begin{aligned}
\Psi = \prod_k [1 + U(1, k) A_k^\dagger + U(2, k) B_k^\dagger \\
+ U(3, k) C_k^\dagger + U(4, k) D_k^\dagger + U(5, k) (W_k^\dagger)] |0\rangle,
\end{aligned} \quad (2)$$

where $|0\rangle$ is the physical vacuum and $U(i, k)$ are variational amplitudes.

Note that with D^\dagger purely imaginary,

$$(A_k^\dagger B_k^\dagger) = (C_k^\dagger C_k^\dagger) = (D_k^\dagger D_k^\dagger) = (W_k^\dagger). \quad (3)$$

Also, the choice of all variational amplitudes $U(i, k)$ as positive is both possible and convenient, assuming that all off-diagonal pairing matrix elements are attractive. Other phase choices are possible for the amplitudes $U(i, k)$. Using $\Psi(+, +, +, +, +)$ to denote a wavefunction in which $U(i, k)$ is positive for all i and k , and, e.g., $\Psi(-, +, +, +, +)$ to denote that $U(1, k)$ is negative for all k ; we find that

$$\begin{aligned}
\Psi(+, +, +, +, +) &= \Psi(-, -, +, +, +) \\
&= \Psi(+, +, -, +, +) = \Psi(+, +, +, -, +) \\
&= \Psi(-, -, -, +, +) = \Psi(-, -, +, -, +) \\
&= \Psi(+, +, -, -, +) = \Psi(-, -, -, -, +).
\end{aligned} \quad (4)$$

By equal, we mean that the projected wavefunctions have overlaps of 1. Within factors of ± 1 , this also holds for the collective states in $N = Z$ and for $N = Z \pm 2n$, in e-e and o-o systems. This is a reflection of the equalities of Eq. (3). However $\Psi(-, -, -, -, -)$ is generally quite different from the wave functions of Eq. (4), as is $\Psi(-, +, +, +, +)$. The identities of Eq. (4) sometimes cause difficulties with an iterative variational procedure, as the trial variational wavefunction can oscillate between the different minima. We find that limiting the magnitude of changes in amplitudes from one iteration to the next is helpful.

The number parity of C^\dagger pairs and D^\dagger pairs, as well as the number parity of the sum of $(A^\dagger + B^\dagger)$ pairs is conserved. This can be seen from the structure of the Hamiltonian and Eq. (3). To classify the number parity of projected states succinctly, we define a Q quantum number. When the number parity of N-P $T = 0$ pairs is even in a projected wavefunction, we call the state $Q = 1$. When the number parity of N-P $T = 0$ pairs is odd, we call the state $Q = 2$. As exact number projection of both protons and neutrons is also enforced in our wavefunctions, this one descriptor is sufficient to specify all number parities in the wavefunctions. In an e-e nucleus, $Q = 1$ means that both the number parity of $T = 0$ and $T = 1$ N-P pairs is even and $Q = 2$ means that both are odd. In an o-o nucleus, $Q = 1$ means that the number parity of $T = 1$ N-P pairs is odd, while $Q = 2$ means that the number parity of $T = 1$ N-P pairs is even.

There is a close relation between number parity projection and the exact parity projection that we have used in studies [16] of octupole correlations. Q -projection, in fact, corresponds exactly to parity projection for octupole correlations, if we take Q as the number parity of odd parity configurations. Our calculations show that the lowest $Q = 1$ and $Q = 2$ states in $N = Z$ o-o nuclei are degenerate when the $T = 0$ and $T = 1$ pairing strengths are the same. This corresponds to the parity doublets [16] calculated and seen in odd mass nuclides.

In the case of $N = Z$ even-even nuclides, the exact ground state is $T = 0$. This condition is satisfied in the quasi-particle method in an average way by the condition $\langle \hat{\mathbf{T}} \rangle = 0$. We do not impose this condition on our wavefunctions. For our variational wavefunctions, bearing in mind the phase of proton wavefunctions, this condition is satisfied when $U(1, k) = U(2, k)$ and

we find that the $Q = 1$ variational solutions for $N = Z$ e-e nuclides satisfy this condition exactly. However, this condition is also satisfied exactly when T is manifestly not equal to 0, e.g., for the lowest energy state in $N = Z$ o-o ($Q = 1$ or 2) and for the lowest $Q = 2$ state in $N = Z$ e-e nuclei.

No assumptions about level degeneracy or pairing matrix elements, are made in our code for N-P pairing. This treatment can be used directly, in the context of the Strutinski method, to determine energy surfaces of nuclei and to carry out low energy structure studies. Here we present sample calculations to illustrate some features of N-P pairing. For simplicity, we use equally spaced single-particle levels and diagonal and off-diagonal matrix elements that are level independent.

Diagonal pairing matrix elements are taken to be twice the size of the off-diagonal ones. This is a fairly realistic choice, suggested by a δ interaction or by a density dependent δ interaction [17] matrix elements and has non-trivial consequences. The magnitude of diagonal matrix elements is significant as the W_k^\dagger configurations associated with $U(5, k)$ are lowered by an amount $(3G_{k,k}^{T=1} + G_{k,k}^{T=0})$, while other configurations are lowered by only $G_{k,k}^{T=1}$ or, in the case of the D_k^\dagger configuration, by $G_{k,k}^{T=0}$. This diagonal energy shift further enhances the amplitude $U(5, k)$; i.e., the ‘alpha correlation’ configuration in the wavefunction. This feature is missing in a quasi-particle description of N-P pairing.

We set

$$G_{i,j}^{T=1} = G_{i,j}^{T=0} = 0.5G_{i,i}^{T=1} = 0.5G_{i,i}^{T=0} = G. \quad (5)$$

Equating the $T = 1$ and $T = 0$ N-P interaction strengths seems realistic for $A \sim 60$ region, since in ^{58}Cu , the $T = 0$ 1^+ state is the ground state and in ^{60}Ga , the $T = 1$ 0^+ state is the ground state. In the model calculations, the single-particle energy level spacing is 1 MeV, $G = 0.3$ MeV, and the system consists of 30 Nilsson levels, each accomodating two protons and two neutrons. In the e-e system we set the number of protons, N_z , equal to 30 and in the o-o system, we set it to 31. We have done calculations with $N_n = 32, 34$ and 36 in the e-e systems and $N_n = 31, 33$ and 35 in the o-o systems. To avoid confusion with the real elements Zn and Ga, we define two imaginary elements; EE for $N_z = 30$ e-e systems and OO for the

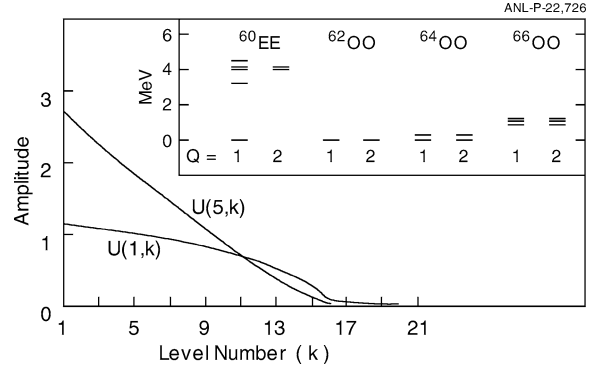


Fig. 1. Ground state amplitudes in ^{60}EE . Further details are given in the text. Low lying states in ^{60}EE , ^{62}OO , ^{64}OO and ^{66}OO are shown in the insert, illustrating the extra degeneracies arising from multiple pairing modes.

$N_z = 31$ o-o systems with the total mass given as a superscript.

In Fig. 1 we plot the ground state amplitudes for ^{60}EE . The normalization is 1.0 for the projected wavefunction. In this variational wavefunction, $U(1, k) = U(2, k)$ and $U(3, k) = U(4, k)$ exactly for all k . In addition, $U(3, k)$ is, within a few %, the same as $U(1, k)$, so we plot only $U(1, k)$ and $U(5, k)$. To better grasp the dominance of the $U(5, k)$ amplitudes, note that $U(5, k)$ should be compared to $U(1, k)^2$ as the $U(5, k)$ configuration has four nucleons while the $U(1, k)$ configuration has only two nucleons. The ‘alpha correlations’ are very enhanced. This groundstate wavefunction appears to be one with little residual interaction effects; i.e., the fermi surface is quite sharp. The amplitude $U(5, 15)$ is 0.14 and the amplitude $U(5, 16)$ is 0.004. Similarly, the amplitude $U(1, 15)$ is 0.29 and $U(1, 16)$ is 0.05. Amplitudes for levels beyond $k = 20$ are not plotted; they are very close to zero.

In Table 1 we present diagonal and off-diagonal correlation energies for several different states. By off-diagonal correlation energy $\langle A^\dagger A \rangle$, we mean $\sum_{i,j \neq i} G_{i,j}^{T=1} \langle A_i^\dagger A_j \rangle$. The relative importance of diagonal correlations can be seen quite clearly. There are several other things to be noted in Table 1. Doing separate variational calculations for $Q = 1$ and $Q = 2$, we get the same energies and the same wavefunctions (apart from the interchange of $U(3, k)$ and $U(4, k)$) in ^{62}OO . The polarizing effects of the N-P pair in ^{62}OO are substantial as can be seen in the in-

Table 1
Correlation energies

	$\langle A^\dagger A \rangle$	$\langle B^\dagger B \rangle$	$\langle C^\dagger C \rangle$	$\langle D^\dagger D \rangle$
$^{60}\text{EE } Q = 1$				
Off-Diagonal (MeV)	3.18	3.18	2.79	2.79
Diagonal (MeV)	8.88	8.88	8.85	8.85
$^{60}\text{EE } Q = 2$				
Off-Diagonal (MeV)	1.84	1.84	3.35	3.35
Diagonal (MeV)	8.32	8.32	8.95	8.95
$^{62}\text{OO } Q = 1$				
Off-Diagonal (MeV)	2.28	2.28	4.67	2.14
Diagonal (MeV)	8.89	8.89	9.55	8.88
$^{62}\text{OO } Q = 2$				
Off-Diagonal (MeV)	2.28	2.28	2.14	4.67
Diagonal (MeV)	8.89	8.89	8.88	9.55
$^{64}\text{EE } Q = 1$				
Off-Diagonal (MeV)	4.12	4.19	1.69	1.69
Diagonal (MeV)	10.15	8.95	8.89	8.89

crease in the corresponding off-diagonal correlation energy. In ^{64}EE , it may seem peculiar that the proton off-diagonal correlation energy is slightly larger than that of the neutrons. This is due to the fact that the number of protons corresponds to an exactly half filled system, while the neutron number goes beyond the half filled system. More interesting, the off-diagonal N-P correlation energy has not disappeared; it is still slightly more than 60% of the value in ^{60}EE . The reason for the persistence of these correlations is that all amplitudes $U(i, k)$ are fed by and feed into $U(5, k)$.

The effect of the strong diagonal correlations becomes apparent when we consider the energies of excited states. One technique, that is very useful for the study of 0+ pairing excitations for like-nucleon $T = 1$ pairing, is the discretized Hill–Wheeler method. In this approach, one varies the pairing interaction strength and generates new wavefunctions for each new value of this strength. The solutions so obtained are then diagonalized using the physical value of the interaction strength and taking into account

Table 2
Amplitudes in $^{60}\text{EE } Q = 2$

	i				
	1	2	3	4	5
$U(i, 15)$	0.04	0.04	0.44	0.05	0.03
$U(i, 16)$	0.03	0.03	0.04	0.33	0.01

non-zero overlaps of the solutions. As our code allows arbitrary pairing strengths, we have implemented this procedure by separately varying $G_{n,n}$, $G_{p,p}$, $G_{n,p}^{T=1}$ and $G_{n,p}^{T=0}$. After diagonalization, this gives excited states at roughly 5 MeV excitation energy in ^{60}EE .

The lowest $Q = 2$ state is at somewhat lower energy, ~ 4 MeV. We can use this $Q = 2$ state to generate several additional states in a very simple way. In Table 2 we show the amplitudes $U(i, 15)$ and $U(i, 16)$ for the $Q = 2$ state. Interchanging $U(3, 15)$ with $U(4, 15)$ and simultaneously interchanging $U(3, 16)$ with $U(4, 16)$ gives another $Q = 2$ state at about the same energy. We can also generate four $Q = 1$ states, at about the same energy. These are obtained by: (1) interchanging $U(3, 15)$ with $U(4, 15)$; (2) interchanging $U(3, 16)$ with $U(4, 16)$; (3) interchanging $U(1, 15)$ with $U(3, 15)$ and $U(2, 16)$ with $U(4, 16)$; (4) interchanging $U(2, 15)$ with $U(3, 15)$ and $U(1, 16)$ with $U(4, 16)$. All of these configurations have the same single-particle energy. After carrying out the interchanges and diagonalizing the resulting projected non-orthogonal wavefunctions, we get two $Q = 2$ states and four $Q = 1$ states near 4 MeV. Finally, interchanging all five amplitudes $U(i, 15)$ with the $U(i, 16)$ amplitudes in the $Q = 1$ groundstate wavefunction gives another useful basis state. When this state is included in the diagonalization, we get a $Q = 1$ state at 3.2 MeV, three $Q = 1$ states at roughly 4 MeV and two $Q = 2$ states at 4 MeV. With an increase of neutron number, the wavefunctions obtained by interchanging rows in the ground state wavefunction play an increasingly important role in determining the $Q = 1$ excited states. The excitation energy of the first $Q = 1$ excited state falls to 2.3 MeV in ^{62}EE .

It has long been thought that N-P transfer reactions provide a clear signal of N-P correlations. As the alpha-particle, $U(5, k)$ amplitudes are so dominant near the $N = Z$ line, the hope of seeing large transfer

Table 3
Amplitudes in ^{66}OO $Q = 1$

	i				
	1	2	3	4	5
$U(i, 16)$	0.49	0.07	0.05	0.04	0.03
$U(i, 17)$	0.39	0.05	0.04	0.03	0.02
$U(i, 18)$	0.04	0.03	0.32	0.02	0.01

cross-sections should be somewhat tempered. We have calculated the N-P spectroscopic factor, defined as

$$S_{N-P}^{T=1} = \left[\langle Z+1, N+1 | \sum_k C_k^\dagger | Z, N \rangle \right]^2 \quad (6)$$

for the $T = 1$ N-P pair transfer. For $T = 0$ transfer, D_k^\dagger replaces C_k^\dagger . As $G^{T=1}$ is the same as $G^{T=0}$, the results are identical for the two types of N-P pair transfer. In our model system, the spectroscopic factors are 8, 5 and 4 for the ^{60}EE , ^{62}EE and ^{64}EE targets, respectively. None are very large, but they do not drop off quickly with increasing neutron number. It may be interesting to carry out deuteron transfer experiments on nuclei that are somewhat removed from the $N = Z$ line and hence available as targets. The spectroscopic factor for neutron pair addition on an ^{60}EE target is 8, as one might expect.

It is important to realize that the state strongly populated in the N-P pair transfer reaction to levels in ^{64}OO and ^{66}OO may not be the ground state. The ground state may be a configuration in which there are odd numbers of nucleons (blocking) in two different Nilsson levels. We plan to extend our variational method to include blocked configurations. Making some crude assumptions for now, we estimate that the state populated in pair transfer is at or near ground in ^{64}OO and at roughly 1 MeV excitation in ^{66}OO .

In odd-odd nuclei with a neutron excess, the degeneracy is very high. This phenomenon of multiple degeneracy is a direct consequence of the multiple pairing correlation modes that are important near the $N = Z$ line. The main features of this new degeneracy can be understood in a very simple way. Consider the amplitudes in the lowest $Q = 1$ state for ^{66}OO , shown in Table 3. In this wavefunction, roughly speaking, the two excess neutron pairs go into levels 16 and 17 and the N-P $T = 1$ pair goes into level 18. How-

ever, there are two other $Q = 1$ configurations with the same total single particle energy; i.e., states in which the N-P $T = 1$ pair goes into either level 16 or 17 and a neutron pair goes into level 18. We approximate one such configuration by interchanging $U(1, 16)$ with $U(3, 16)$ and simultaneously interchanging $U(1, 18)$ with $U(3, 18)$. Another such configuration is obtained by making the interchanges in level 17 rather than 16. In leading order, the three wavefunctions are orthogonal and the interaction matrix element vanishes. In higher order, they have non-zero overlaps and non-zero interaction matrix elements which we have taken into account. After diagonalization, one of the states gets pushed down by 250 keV.

In addition to this new degeneracy, we have the expected degeneracy associated with the $Q = 2$ levels. The $Q = 2$ states in ^{66}OO have exactly the same spectrum as the $Q = 1$ states. This gives a degeneracy of six at an estimated excitation energy of 1 MeV. In ^{64}OO , we estimate that the lower of two $Q = 1$ states will be at or near ground and the relevant diagonalization again gives a second state 0.25 MeV above it. Each has a $Q = 2$ degenerate partner, giving a total degeneracy of four. The calculated splittings do depend on the magnitude of the pairing interaction strength. We show these spectra, as well as that of ^{60}EE , as the insert in Fig. 1.

In summary, we have developed variational wavefunctions for the simultaneous treatment of N-P pairing in the $T = 1$ and $T = 0$ channels that explicitly include alpha-like correlations and allow for arbitrary single-particle energy level spacings. We have developed a triple projection before variation procedure for determining these wavefunctions. Utilizing a model system with equally spaced single-particle levels, we have calculated several features of nuclei near the $N = Z$ line. Using amplitude interchanges to construct basis states, in a framework of configuration interaction calculations, we find a new phenomenon of multiple degeneracy in the low-lying states of odd-odd nuclei, and this same phenomenon at somewhat higher excitation energy in e-e nuclei.

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